

The Statistics of Chaotic Tunnelling

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We discuss the statistics of tunnelling rates in the presence of chaotic classical dynamics. This applies to resonance widths in chaotic metastable wells and to tunnelling splittings in chaotic symmetric double wells. The theory is based on using the properties of a semiclassical tunnelling operator together with random matrix theory arguments about wave function overlaps. The resulting distribution depends on the stability of a specific tunnelling orbit and is therefore not universal. However it does reduce to the universal Porter-Thomas form as the orbit becomes very unstable. For some choices of system parameters there are systematic deviations which we explain in terms of scarring of certain real periodic orbits. The theory is tested in a model symmetric double well problem and possible experimental realisations are discussed.

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Tunnelling is crucial in describing many physical phenomena, from chemical and nuclear reactions to conductances in mesoscopic devices and ionisation rates in atomic systems. When such systems are complex, it is natural to model tunnelling effects using random matrix theory [1]. We show here that when the underlying system is one of clean chaotic dynamics, successful statistical modelling demands explicit incorporation of nonuniversal, but simple, dynamical information. We derive a distribution for the tunnelling rate which depends on a single parameter, calculated from the stability properties of the dominant tunnelling orbit.

The signatures of chaos in tunnelling rates have been receiving a growing amount of attention, two important regimes having been considered. The first is that the quantum state is initially localised in a region where the dynamics is largely nonchaotic and one wants to understand the tunnelling rate through chaotic regions of phase space [2–4]. The second, and the one we shall focus on, is that virtually all of the energetically accessible phase space is chaotic [5,6] so that the quantum state is initially localised in a chaotic region of phase space. These two situations are different in many important ways. In particular, the statistical distribution of the tunnelling rates in the first regime has power law decays [3] whereas we show that the distribution in the second regime has exponential decay. The result is a generalisation of the Porter-Thomas distribution [7] used to model neutron and proton resonances [7–9] and conductance peak heights in quantum dots [10,11].

It is shown in Refs. [5] that the average tunnelling rate from an energetically-connected region of phase space is determined by a complex orbit we will call the instanton. Fluctuations about this average appear to be pseudorandom in the chaotic case and are given by properties of the wavefunction in an area localised around a real extension of the instanton [6]. To characterise these fluctuations we define a rescaled tunnelling rate as follows.

In the case of metastable wells the absolute tunnelling rate of a given state labelled by n is measured by the resonance width, or inverse lifetime Γ_n . The corresponding normalised tunnelling rate is defined to be

$$y_n = \Gamma_n / \bar{\Gamma}, \quad (1)$$

where $\bar{\Gamma}(E, \hbar) = \langle \Gamma_n \rangle$ is a local average computed for a given set of physical parameters. $\bar{\Gamma}(E, \hbar)$ is a smooth, monotonic function of its arguments and is given by an explicit formula in terms of the (purely imaginary) action and stability of the instanton [5]. A similar definition holds for splittings in double wells and in either case $\langle y_n \rangle = 1$ by construction.

Fluctuations in y_n are calculated using a *tunnelling operator*, \mathcal{T} , which is constructed from the semiclassical Green's function and can be interpreted as transporting the wavefunction across the barrier. Specifically,

$$y_n \propto \langle n | \mathcal{T} | n \rangle, \quad (2)$$

where $|n\rangle$ is the wavefunction (which may be calculated while ignoring tunnelling effects) represented in a Hilbert space which quantises a surface of section. A closed-form expression can be found by expanding classical actions in quadratic order around the instanton. Details can be found in [6], but for present purposes it is enough to know its spectrum. For a two-dimensional system this is $\{\lambda^k |\lambda|^{1/2}, k = 0, 1, \dots\}$, where λ is the inverse of the stability of the instanton orbit, is always less than unity in magnitude and can easily be found using real dynamics in the inverted potential. (The discussion is readily generalised to higher dimension but we refrain from doing so for clarity.) To derive statistical distributions for y_n , we will make statistical assumptions about the state $|n\rangle$, but not about the tunnelling operator. The resulting distribution depends parametrically on λ and is therefore system-specific and not universal.

We can always express \mathcal{T} as a diagonal operator in its own eigenbasis: $\sum_k \lambda^k |\lambda|^{1/2} |k\rangle\langle k|$. We then have

$$y_n = a \sum_{k=0}^{\infty} \lambda^k |\langle k|n\rangle|^2 = a \sum_{k=0}^{\infty} \lambda^k |x_k|^2 \quad (3)$$

where we denote $x_k = \langle k|n\rangle$ and the prefactor $a = 1 - \lambda$ ensures that $\langle y \rangle = 1$. The states $|n\rangle$ are normalised so that on average $|x_k|^2$ is unity. We now make the statistical ansatz that the overlaps can be treated as Gaussian random variables. This is the basis of almost all statistical treatments of wave functions, going back to the seminal work of Porter and Thomas [7]. In the event that there is a time reversal symmetry, x_k can be expressed as a single real number, leading to GOE statistics. If there is no such symmetry then x_k is complex and will be described by two statistically independent quantities leading to GUE statistics.

We simplify the derivation by assuming GOE statistics; the generalisation to GUE is simple and we give the final result for both. We start by assuming that the x_k are statistically independent and given by the joint distribution $P(\mathbf{x})d\mathbf{x} = \prod_k [\exp(-x_k^2/2)/\sqrt{2\pi}] dx_k$ where $\mathbf{x} = \{x_k\}$. We then note that

$$P(y; \lambda) = \int d\mathbf{x} P(\mathbf{x}) \delta\left(y - a \sum_{k=0}^{\infty} \lambda^k x_k^2\right). \quad (4)$$

We use the identity $\delta(z) = \int dt \exp(itz)/2\pi$ in the above expression and observe that each x_k involves a simple Gaussian integral. The final result (and generalising to the GUE case) is

$$P(y; \lambda) = \frac{1}{2\pi} \int dt e^{ity} \prod_{k=0}^{\infty} \left(1 + \frac{2i}{\beta} a \lambda^k t\right)^{-\beta/2}, \quad (5)$$

where $\beta = 1$ and 2 for GOE and GUE respectively. The product above converges rapidly provided λ is not too close to unity so the formula can easily be used to calculate $P(y; \lambda)$ in practice.

This result has a simple interpretation if we think of each eigenstate of \mathcal{T} as providing a distinct and statistically independent channel to tunnel; it then corresponds to the discussion of Ref. [12] but with an infinite number of distinctly weighted open channels. We could even imagine adding a weak magnetic field so as to interpolate between the GOE and GUE limits as in [13] although we refrain from that here. As mentioned, we have $\langle y \rangle = 1$ by construction; the second moment is

$$\langle y^2 \rangle = 1 + \frac{2}{\beta} \frac{1 - \lambda}{1 + \lambda}. \quad (6)$$

The channel interpretation helps in a qualitative understanding of this distribution as we vary λ . For small λ , only the first ($k = 0$) channel plays any significant

role and the distribution is of the Porter-Thomas form: $\exp(-y/2)/\sqrt{2\pi y}$ and $\exp(-y)$ for $\beta = 1$ and 2 respectively. This can be understood analytically from (5) by doing a branch-point/residue analysis around the nearest singularity at $t = i\beta/2a$. This distribution is commonly used to model point tunnelling contacts [10,12,13]. It is often a very accurate approximation but its validity is not universally guaranteed, as we shall discuss. For λ close to unity, many channels contribute significantly, the fluctuations around the mean are accordingly reduced and the distribution approaches a Gaussian with variance $\sigma^2 \approx a/\beta$ (which becomes a delta function for small a).

For $\lambda > 0$ and $y \leq 0$ we close the contour of (5) in the lower half plane; since the integrand has no singularities there, the result is simply zero. This is consistent with the fact that \mathcal{T} is a positive definite operator so that Eq.(3) does not admit the possibility of negative y . By the same argument, any derivative of $p(y)$ is also zero for $y \leq 0$ implying a nonanalyticity at $y = 0$ with $p(y)$ going to zero faster than any power of y for y small and positive. In the opposite limit $y \gg \lambda$ we can expand around the first singularity to obtain

$$\begin{aligned} P(y; \lambda)_{\text{GOE}} &\approx \frac{\exp(-y/2a)}{\sqrt{2\pi a y}} \\ P(y; \lambda)_{\text{GUE}} &\approx \frac{\exp(-y/a)}{a}. \end{aligned} \quad (7)$$

This falls off exponentially with y , and not with a power law as observed in the chaos-assisted regime [3].

Equations (3), (5) and (6) remain valid when λ is negative. This situation arises when we compute splittings in symmetric double wells for which the symmetry is inversion through a point rather than reflection through an axis [6]. In this situation \mathcal{T} is no longer positive definite and we admit the possibility of negative splittings (for which the odd member of a doublet has a lower energy than the even member). The distribution then allows all values of y , positive and negative. It decays exponentially for $|y| \gg \lambda$ as in Eq. (7) but with different exponents for $y > 0$ and $y < 0$ because on doing the integral (5) we must switch from closing the integration contour in the lower half plane to the upper half plane as y changes sign. For a given state, we can typically induce a zero splitting by tuning one system parameter. A zero splitting means that we can construct states which remain localised in either well for all time as in the one dimensional time-dependent system considered in [14].

At this point we contrast our results with standard random matrix theory modelling. In section VII.H of their extensive review [8], Brody et al. show under rather general assumptions that one expects a Gaussian distribution for the expectation values of an arbitrary operator by showing that all of the moments of the distribution approach those of a Gaussian. This can be understood as a sort of central limit theorem. One of their assumptions is

that the operator is non-singular, *i.e.* does not have many zero eigenvalues. Because of the exponential decay of the eigenvalues of the tunnelling operator \mathcal{T} , it is effectively singular. Therefore their conclusions do not apply to our situation and we have non-Gaussian distributions. It is interesting to note that in the limit $|\lambda| \rightarrow 1$, the operator \mathcal{T} has an ever increasing number of significant eigenvalues and the distributions do in fact approach Gaussians, in conformity with their general considerations.

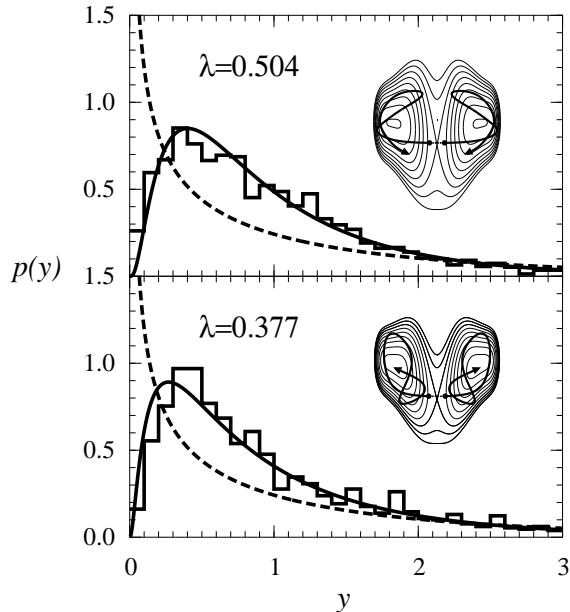


FIG. 1. Results for two typical potentials, with $(\mu, \nu, \sigma) = (0.15, 0.17, 0.00)$ above and $(0.25, 0.50, 0.00)$ below. In both cases the energy is lower than saddle maximum by an amount 0.1. The continuous curves are the theoretical distributions calculated using the appropriate values of λ (shown). The dashed curves show the Porter-Thomas distribution for comparison. The insets show the corresponding instanton orbits and their real extensions.

Since it is a simpler numerical task to calculate many splittings in a double well than to calculate many resonance widths in a metastable well, we use the former to test our predictions and note that any conclusions apply identically to the latter. Consider the potential

$$V(x, y) = (x^2 - 1)^4 + x^2 y^2 + \mu y^2 + \nu y + \sigma x^2 y. \quad (8)$$

There is a reflection symmetry in x and if the energy is less than $1 - \nu^2/4\mu$ the motion is classically confined either to $x < 0$ or to $x > 0$. It is convenient to work at fixed energy in order to keep λ constant and we do this by quantising $q = 1/\hbar$ [6], that is, by finding those values of \hbar which are consistent with a specified choice of parameters and energy. This is effectively what happens, for example, in scaling problems such as a hydrogen atom in a magnetic and electric field [15]. In Fig. 1 we show histograms constructed from the q -spectra for two choices

of parameters such that the classical dynamics is almost fully chaotic. We also show the distribution (5) with $\beta = 1$ and using the corresponding values of λ . Clearly, the numerically computed histograms are well captured by the theoretical distribution. We show, for comparison, the Porter-Thomas distribution which clearly fails to correctly model the numerical data. We remark that this sort of agreement was observed for most parameter values as long as the dynamics was fully chaotic.

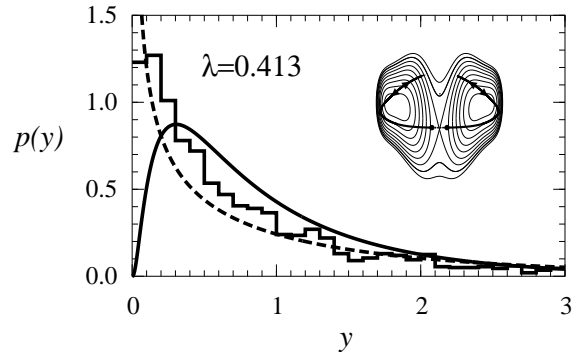


FIG. 2. As in Fig. 1 but for parameter values $(\mu, \nu, \sigma) = (0.25, 0.40, 0.254)$ for which the real extension of the instanton orbit is periodic and the resulting distribution is significantly different from the RMT prediction.

In Fig. 2 we show an exception to the general agreement. In this case the numerical histogram is intermediate between the theoretical distribution (5) and the Porter-Thomas form. We attribute this to the effects of scarring [16,17], as follows. The instanton has real turning points where the momentum vanishes and the position is real. At these points we can elect either to integrate in imaginary time in which case the instanton retraces itself or to integrate in real time, in which case we get a real trajectory. We refer to this real trajectory as the real extension of the instanton. There is no reason why this real extension should itself be periodic. Typically it is not. However, the parameters of Fig. 2 have been tuned so that the real extension is in fact periodic. We find in this case that the overlaps $x_k = \langle k|n \rangle$ are no longer distributed according to the Gaussian $P(x_k) = \exp(-x_k^2/2)/\sqrt{2\pi}$ as assumed in our derivation — there are relatively more large overlaps and more small overlaps. This effect can be explained using a recent theory of scarring [17] which describes how the overlaps between a wavepacket placed on a periodic orbit and the chaotic eigenstates deviate from random matrix theory. In our problem the eigenvectors $|k\rangle$ behave like wavepackets of this type when the real extension is periodic. The effect of this deviation from random matrix theory is to give more large splittings and more small splittings than (5) predicts and, therefore, to push the distribution in the direction of the Porter-Thomas form.

We remark that for $\nu = \sigma = 0$, the real extension is always a periodic orbit [5] and we see anomalous statistics for this situation as well.

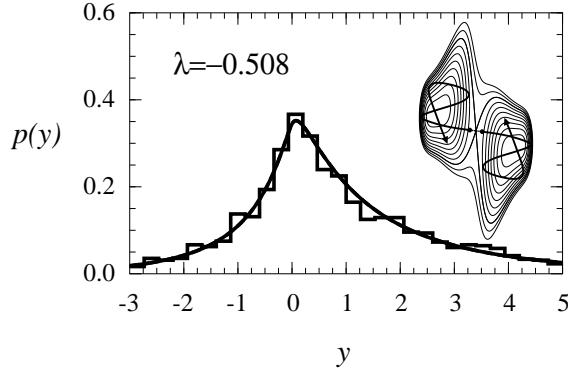


FIG. 3. Results for the inversion-symmetric potential with $(\mu, \tau) = (0.1, 1.0)$ for which zero and negative splittings are allowed.

The final case we discuss is if the term $\nu y + \sigma x^2 y$ in (8) is replaced by τxy . Now the potential is symmetric under $(x, y) \rightarrow (-x, -y)$ rather than under $(x, y) \rightarrow (-x, y)$ (this symmetry would persist if we were to add a uniform magnetic field). In this case $\lambda < 0$ [6] and negative splittings can occur. We present the results for a typical case in Fig. 3. Again, the theoretical distribution agrees with the histogram.

Our results are relevant to situations in which particles tunnel out of or between chaotic regions separated by an energetic barrier. Applications include hydrogen atoms in parallel electric and magnetic fields where the competition between the imposed fields and the Coulomb force causes chaotic motion while the presence of the electric field causes tunnelling [15]. Dissociative decays of excited nuclei and molecules may also fall into this regime.

Another application is to conductances of quantum dots. In the Coulomb blockade regime electrons must tunnel into and out of dots which are thought to be chaotic. Such experiments have been done [11] leading to results which are consistent with the Porter-Thomas distribution for the tunnelling widths, just as for the neutron and proton resonance widths. We contend that the reason is that the instanton path in all cases is very unstable, leading to a small value of λ . For energies near the saddle $\lambda \approx \exp(-2\pi\omega_y/\omega_x)$ [18] where ω_x and ω_y are the curvatures of the potential saddle along and transverse to the instanton, respectively. This is often small, but by making the saddle flat in the transverse direction or sharp in the instanton direction, it is possible to have λ be of order unity. It is an interesting question whether this can be arranged for the quantum dots. One feature which helps in this regard is that we predict a distribution which vanishes for small y whereas the Porter-Thomas distribution diverges as $1/\sqrt{y}$. This difference could be

discernible even for rather small values of λ .

Another possibility for nonuniversal statistics would be a situation analogous to Fig. 2, where the tunnelling route is directly connected to a real periodic orbit. This geometry could be engineered into quantum dots and is present in the hydrogen atom problem [15]. In this case we predict deviation from the predictions of random matrix theory. This would be similar in spirit to the recent work of Narimanov et al. [19] who look for dynamical effects in the correlations of conductance peaks of quantum dots.

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